Sets of Fourier Coefficients using Numerical Quadrature*

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One approach to the calculation of Fourier trigonometric coefficients $\hat{f}(r)$ of a given function $f(x)$ is to apply the trapezoidal quadrature rule to the integral representation

$$\hat{f}(r) = \int_0^1 f(x)\mathrm{e}^{-2\pi irx}dx.$$

Some of the difficulties in this approach are discussed. A possible way of overcoming many of these is by means of a "subtraction" function. Thus, one sets

$$f(x) = h_{p-1}(x) + g_p(x),$$

where $h_{p-1}(x)$ is an algebraic polynomial of degree $p-1$, specified in such a way that the Fourier series of $g_p(x)$ converges more rapidly than that of $f(x)$. To obtain the Fourier coefficients of $f(x)$, one uses an analytic expressionfor those of $h_{p-1}(x)$ and numerical quadrature to approximate those of $g_p(x)$.

*This work was supported in part by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Advanced Scientific Computing Research, U.S. Dept. of Energy, under Contract W-31-109-Eng-38

PART 1: FOURIER SERIES

A Few Classical Results

of a

Straightforward Nature

Fourier series over [0,1] for $g(x)$.

$$\bar{g}(x) = \sum_{\ell=-\infty}^{\infty} \hat{g}(\ell) \mathrm{e}^{2\pi i \ell x}$$

$$\hat{g}(r) = \int_0^1 g(x) \mathrm{e}^{-2\pi i r x} dx$$

$$\begin{aligned}\bar{f}(x) = a_0 \quad &+ \quad a_1 \cos 2\pi x + a_2 \cos 4\pi x + \dots \\ &+ \quad b_1 \sin 2\pi x + b_2 \sin 4\pi x + \dots\end{aligned}$$

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Example 1: $f(x) = \mathrm{e}^{\alpha x}/(\mathrm{e}^{\alpha} - 1)$ $\qquad \alpha = \frac{4\pi^2}{10} \simeq 3,6$

$a_0 \simeq 0.3$

$a_{10} = 10^{-3} \quad a_{100} = 10^{-5} \qquad a_{1000} = 10^{-7}$

$b_{100} = 1.3 \times 10^{-3} \quad b_{1000} = 1.3 \times 10^{-4}$

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Example 2: $f(x) = \frac{1-\rho^2}{1-2\rho\cos 2\pi x - \rho^2}$ $\qquad \rho = \frac{1}{\sqrt{10}} = 0.32$

$a_0 = 1 \quad a_1 = 0.32 \qquad a_2 = 0.1 \quad a_3 = 0.032 \quad a_4 = 0.01$

$a_5 = 0.0032 \qquad a_8 = 0.0001$

$a_{12} = 10^{-6}$

$a_{16} = 10^{-8}$

$b_j = 0$

$f(x)$ is $C^\infty[0,1]$ and bounded variation.

(0) Under these circumstances the Fourier series converges

$$\hat{f}(r) \to 0$$

(1) Example 1

$$f(x) = \frac{\mathrm{e}^{\alpha x}}{\mathrm{e}^{\alpha} - 1}; \quad \hat{f}(r) = \frac{\alpha - 2\pi i r}{\alpha^2 + 4\pi^2 r^2}$$

[Cosine coeffts (real part) $\sim O(r^{-2})$. $\alpha = 2$. First 300 coeffts exceed 10^{-6}.]

(2) Example 2

$$f(x) = \frac{1 - \rho^2}{1 - 2\rho\cos 2\pi x + \rho^2}; \quad \hat{f}(r) = \rho^r; \quad |\rho| < 1$$

[$\rho = \frac{1}{2}$; coefficients after $r = 20$ are less than 10^{-6}.]

Any pattern?

FCAE

$$\begin{aligned}\widehat{f}(r) &= -\frac{f(1)-f(0)}{2\pi i r} - \frac{f'(1)-f'(0)}{(2\pi i r)^2} - \cdots \\ &\quad \cdots - \frac{f^{(p-1)}(1)-f^{(p-1)}(0)}{(2\pi i r)^p} + \frac{1}{(2\pi i r)^p}\widehat{f}^{(p)}(r).\end{aligned}$$

Generally, $\widehat{f}(r) = O(r^{-1})$.

GOOD NEWS: When $f^{(s)}(1) = f^{(s)}(0) \quad s = 0, 1, \ldots, p-1$, then $\widehat{f}(r) = O(r^{-p})$.

BETTER STILL: When $f(x)$ is periodic with period 1, then $\widehat{f}(r) = O(r^{-p})$ for all p.

BEWARE: FCAE is generally divergent and is generally NOT
semi-convergent.

WORSE: It can CONVERGE to WRONG limit. When $\phi(x)$ is periodic, the FCAE for $\widehat{f}(r)$ coincides with the FCAE for $(\widehat{f}(r) + \widehat{\phi}(r))$.

FCAE

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PART 2: FFT Approach

FAST FOURIER TRANSFORM

(Beloved of Engineers and others)

Denote the m-panel trapezoidal rule approximation to $I_x(\psi(x)) = I\psi$ by

$$R_x^{[m]}(\psi(x)) = R^{[m]}\psi = \frac{1}{m}\sum_{j=1}^{m} \bar{\psi}(j/m).$$

Recall $\hat{f}(r) = I_x\left(f(x)\mathrm{e}^{-2\pi i r x}\right)$. Introduce to DISCRETE FOURIER COEFFICIENT

$$\begin{aligned} \hat{f}^{[m]}(r) &= R_x^{[m]}\left(f(x)\mathrm{e}^{-2\pi i r x}\right) \\ &= \frac{1}{m}\sum_{j=1}^{m} \mathrm{e}^{-2\pi i j r/m}\bar{f}(j/m) \end{aligned}$$

The FAST FOURIER TRANSFORM

m linear equations $r \in \left[-\frac{m-1}{2}, \frac{m}{2}\right]$ of form $\hat{f} = A\bar{f}$.

A has well-defined structure.

Matrix multiplication can be effected in order $m \log m$ operations instead of order m^2 operations.

Aliasing Formula

$$
\begin{aligned}
\widehat{f}^{[m]}(r) &= \widehat{f}(r) + \widehat{f}(r+m) + \widehat{f}(r+2m) + \ldots \\
&\quad + \widehat{f}(r-m) + \widehat{f}(r-2m) + \ldots \\
&= \sum_{k=-\infty}^{\infty} \widehat{f}(r+km)
\end{aligned}
$$

confirms $\widehat{f}^{[m]}(r)$ is periodic, i.e., $\widehat{f}^{[m]}(r) = \widehat{f}^{[m]}(r+m)$.

$\widehat{f}(r)$ is NOT periodic, but approaches zero.

Some of the Discrete Fourier Coefficients are coefficients of the interpolating Trigonometric Polynomial. Thus, set

$$\widehat{\phi}^{[m]}(r) = \widehat{f}^{[m]}(r) \qquad |r| < m/2$$

$$\widehat{\phi}^{[m]}(r) = \tfrac{1}{2}\widehat{f}^{[m]}(r) \quad r = \pm m/2$$

$$\widehat{\phi}^{[m]}(r) = 0 \qquad\qquad |r| > m/2$$

INTERPOLATING TRIGONOMETRIC POLYNOMIAL is

$$f^{[m]}(x) = \sum_{r=-\infty}^{\infty} \widehat{\phi}^{[m]}(r)\mathrm{e}^{-2\pi irx} = \sum_{|r|\le m/2}{}' \, \widehat{f}^{[m]}(r)\mathrm{e}^{-2\pi irx}$$

Properties:

$$f^{[m]}(x) = \bar{f}(x) \quad x = j/m$$

$$|f^{[m]}(x) - \bar{f}(x)| \le 2 \sum_{|r|>m/2} \widehat{f}(r)$$

SUMMARY

$f(x)$ is our original function.

$\hat{f}(r)$ is the r-th Fourier coefficient of $f(x)$.

$\hat{f}^{[m]}(r)$ is an approximation to this Fourier coefficient using the m-panel trapezoidal rule. This is cyclic, i.e., $\hat{f}^{[m]}(r+m) = \hat{f}^{[m]}(r)$.

$\hat{\phi}^{[m]}(r)$ is essentially the <u>useful</u> subset of $f^{[m]}(r)$, that is,

$$\begin{array}{ll} \hat{\phi}^{[m]}(r) = f^{[m]}(r) & |r| < m/2 \\ \hat{\phi}^{[m]}(r) = \frac{1}{2} f^{[m]}(r) & |r| = m/2 \\ \hat{\phi}^{[m]}(r) = 0 & |r| > m/2 \end{array}$$

$f^{[m]}(x)$ is the interpolating trigonometric polynomial of degree $m/2$. Constructed from the useful subset $\hat{\phi}^{[m]}(r)$.

$$f^{[m]}(x) = \sum_{\text{all} r} \hat{\phi}^{[m]}(r) \mathrm{e}^{2\pi i r x} = \sum_{r \le m/2}{}' \hat{f}^{[m]}(r) \mathrm{e}^{2\pi i r x}$$

PART 3. FCAE

Fourier Coefficient Asymptotic Expansion

Integrate by parts to obtain

$$
\begin{aligned}
\widehat{f}(r) &= \int_0^1 f(x)\mathrm{e}^{-2\pi irx}dx \\
&= \left.\frac{f(x)\mathrm{e}^{-2\pi irx}}{-2\pi ir}\right|_0^1 - \int_0^1 \frac{f'(x)\mathrm{e}^{-2\pi irx}}{-2\pi ir}dx \\
&= -\frac{f(1)-f(0)}{2\pi ir} + \frac{1}{2\pi ir}\,\widehat{f'}(r)
\end{aligned}
$$

Iterate to obtain

$$
\begin{aligned}
\widehat{f}(r) &= -\frac{f(1)-f(0)}{2\pi ir} - \frac{f'(1)-f'(0)}{(2\pi ir)^2} - \cdots \\
&\quad \cdots - \frac{f^{(p-1)}(1)-f^{(p-1)}(0)}{(2\pi ir)^p} + \frac{1}{(2\pi ir)^p}\,\widehat{f^{(p)}}(r).
\end{aligned}
$$

This is the FCAE: Fourier Coefficient Asymptotic Expansion

FCAE

$$\begin{aligned}\widehat{f}(r) &= -\frac{f(1)-f(0)}{2\pi i r} - \frac{f'(1)-f'(0)}{(2\pi i r)^2} - \cdots \\ &\cdots - \frac{f^{(p-1)}(1)-f^{(p-1)}(0)}{(2\pi i r)^p} + \frac{1}{(2\pi i r)^p}\widehat{f}^{(p)}(r).\end{aligned}$$

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PART 4

Joint Approach

combining the good features of the

FCAE and the FFT

FCAE

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Subtract out linear trend

$$f(x) =$$
$$(f(1)-f(0))(x-\frac{1}{2}) + (f(x) - (f(1)-f(0))(x-\frac{1}{2}))$$

$$= h_1(x) + g_2(x)$$

$$\begin{aligned}\widehat{f}(r) &= \widehat{h}_1(r) + \widehat{g}_2(r) \\ &\sim \widehat{h}_1(r) + \widehat{g}_2^{[m]}(r) = \widehat{F}_1^{\{m\}}(r)\end{aligned}$$

Iterate

$$f(x) = h_{p-1}(x) + g_p(x)$$

$$h_{p-1}(x) = \sum_{q=1}^{p-1} \lambda_q B_q(x)/q!$$

where $\lambda_q = (f^{(q-1)}(1) - f^{(q-1)}(0))$. This is a KNOWN polynomial of degree $p-1$.

$$\begin{aligned} \hat{h}_{p-1}(r) &= \sum_{q=1}^{p-1} \lambda_q \hat{B}_q(r)/q! \\ &= \sum_{q=1}^{p-1} \lambda_q/(2\pi i r)^q \end{aligned}$$

On the other hand,

$$g_p(x) \quad = \quad f(x) - h_{p-1}(x)$$

is a function one can evaluate at any abscissa x. It satisfies

$$g_p^{(s)}(1) - g_p^{(s)}(0) = 0 \qquad\qquad s = 0, 1, \ldots, p-1$$

and so

$$\hat{g}_p(r) = O(r^{-p})$$

Part 1	Theoretic Approach
Part 2	FFT Approach
Part 3	FCAE
Part 4	Combined Approach

Other Parts:

- Examples of accuracy of numerical process.
- Given p, m, how to estimate accuracy of numerical result.
- How to update p, m during numerical process to obtain preset absolute accuracy ϵ.
- Successively inaccurate derivatives. No need to compromise numerical integrity.

References J.N.L. LYNESS@MCS.ANL.GOV

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